Noiseless particles with deformable shapes

Martin Campos Pinto (LBNL and CNRS, France)

—

joint work with Alex Friedman, Steve Lund, Dave Grote (LBNL and LLNL)
and Eric Sonnendrücker (University of Strasbourg, France)

LBNL

Berkeley, July 29, 2011

Outline

Outline

1. Introduction
2. Three approaches for particle methods
3. Illustration with a mismatched thermal sheet-beam
4. A theoretical convergence result
5. Conclusion, questions

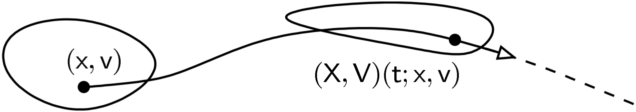
Transport equations with smooth flows

- Transport equation in phase space $\boldsymbol{x} = (x, v) \in \mathbb{R}^d$

$$\{\partial_t + v \cdot \nabla_x + \mathcal{F}(t, x) \cdot \nabla_v\} f(x, v, t) = 0$$

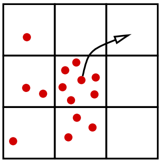
▷ Smooth, reversible characteristic flow $F^n : (x, v) \mapsto (X, V)(t^{n+1})$ where

$$\begin{cases} X'(t) = V(t) \\ V'(t) = \mathcal{F}(t, X(t)) \end{cases} \qquad \text{with} \qquad (X, V)(t^n) = (x, v)$$



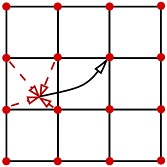
- Vlasov-Poisson : $\mathcal{F} = E = -\nabla\phi$ with $\Delta\phi = \int f \,\mathrm{d}v$ (in arbitrary units)

Numerical methods for the Vlasov equation



$\{(x_i(t), v_i(t)) : i \leq N\}$

$\{f_i(t) : i \leq N\}$

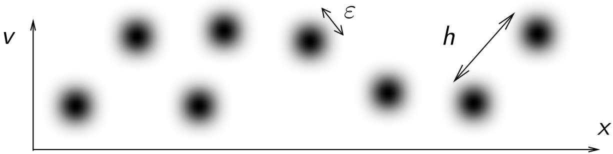


- Particle-In-Cell (PIC) methods (Harlow 1955)
  - physics : (Hockney and Eastwood, 1988), (Birdsall and Langdon, 1991), ...
  - mathematical analysis : (Neunzert and Wick, 1979), (Cottet and Raviart, 1984), (Victory and Allen, 1991), (Cohen and Perthame, 2000), ...
- Eulerian (grid-based) or hybrid methods
  - Forward semi-Lagrangian (Denavit, 1972), (Sonnendrücker and Respaud, 2010), ...
  - Backward semi-Lagrangian (Cheng-Knorr, 1976), (Sonnendrücker, Roche, Bertrand and Ghizzo, 1998), ...
  - Conservative flux based methods (Boris and Book, 1976), (Fijalkow, 1999), (Filbet, Sonnendrücker, Bertrand, 2001), ...
  - Energy conserving FD Method : (Filbet, Sonnendrücker 2003), ...
  - ...

Outline

The standard : particles with (smoothing) scale ε

$$f(\boldsymbol{x}, t^n) \approx f^n_{h,\varepsilon}(\boldsymbol{x}) = \sum_k w_k \varphi_\varepsilon(\boldsymbol{x} - \boldsymbol{x}^n_k) \qquad \begin{cases} h: & \text{distance between particles} \\ \varepsilon: & \text{scale of the particles} \end{cases}$$



- Initialization : particles' centers are either
  - located on regular grid : $x^0_k := (k_0, k_1)h$ with $k \in \mathbb{Z}^d$
  - (pseudo-) randomly distributed with uniform probability, $h \sim N_p^{-1/d}$
  - (pseudo-) randomly distributed with probability f^0 (no h, then)

▷ Set the weights as $w_k := \int_{V_h(x^0_k)} f^0 \approx h^d f^0(\boldsymbol{x}^0_k)$ or $w_k = \mathrm{const} \sim N_p^{-1}$

- Transport : push the centers forward

$$\boldsymbol{x}^{n+1}_k = F^n(\boldsymbol{x}^n_k) \qquad \text{where} \qquad F^n \approx \text{characteristic flow}$$

e.g., $F^n(x, v) = (x + \Delta t v, v + \Delta t E^n(x))$ for Vlasov-Poisson, explicit Euler.

The hybrid : particles with remappings (Denavit, FSL)

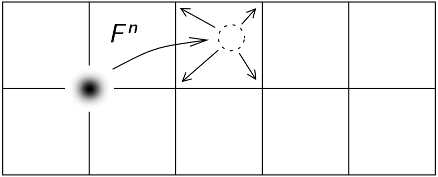
$$f_h^n(\boldsymbol{x}) = \sum_k w_k^n \varphi_h(\boldsymbol{x} - \boldsymbol{x}_k), \quad \text{h} : \begin{cases} \text{distance between particles } (x_k = hk) \\ \text{scale of the particles} \end{cases}$$

(1) Transport as above : push $x_k^{n+1} = F^n(x_k)$,

$$f_h^n(\boldsymbol{x}) \mapsto \tilde{f}_h^{n+1}(\boldsymbol{x}) = \sum_k w_k^n \varphi_h(\boldsymbol{x} - \boldsymbol{x}_k^{n+1})$$

(2) Remap with standard interpolation scheme : compute $w_k^{n+1} = w_k(\tilde{f}_h^{n+1})$

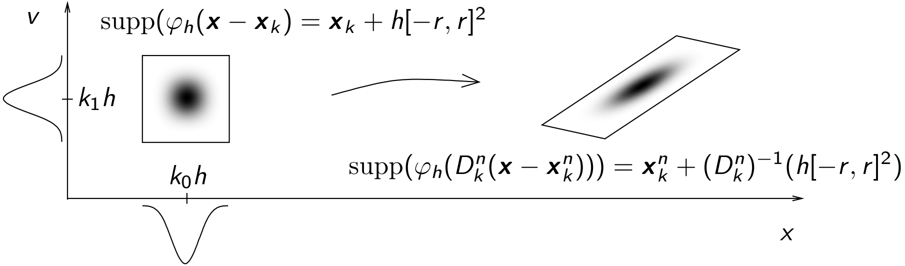
$$\tilde{f}_h^{n+1}(\boldsymbol{x}) \mapsto f_h^{n+1}(\boldsymbol{x}) = \sum_k w_k^{n+1} \varphi_h(\boldsymbol{x} - \boldsymbol{x}_k)$$



The (not so) new : particles with deformations

Each particle has a weight w_k^n, center $x_k^n \in \mathbb{R}^d$ and $d \times d$ deformation matrix D_k^n

$$f_h^n(\boldsymbol{x}) = \sum_k w_k^n \varphi_h(D_k^n(\boldsymbol{x} - \boldsymbol{x}_k^n))$$



▷ see previous methods by (Thomas Hou, 1990), (Bateson and Hewett, 1998), (Cohen and Perthame, 2000), (Cottet, Koumoutsakos and Salihi, 2000), (Hewett, 2003), (Bergdorf, Koumoutsakos 2006) ... list not exhaustive !

How to deform the particles along the flow

- reversible flow $F^n \implies$ exact transport reads

$$\varphi_h(\boldsymbol{x} - \boldsymbol{x}_k^n) \mapsto \varphi_h((F^n)^{-1}(\boldsymbol{x}) - \boldsymbol{x}_k^n)$$

- first order expansion with Jacobian matrices $J_F(\boldsymbol{x}) = \big(\partial_j F_i(\boldsymbol{x})\big)_{1\le i,j\le d}$

$$(F^n)^{-1}(\boldsymbol{x}) \approx \boldsymbol{x}_k^n + J_{(F^n)^{-1}}(\boldsymbol{x}_k^{n+1})(\boldsymbol{x} - \boldsymbol{x}_k^{n+1})$$

▷ deform the particles with

$$\varphi_h(D_k^n(\boldsymbol{x} - \boldsymbol{x}_k^n)) \mapsto \varphi_h(D_k^{n+1}(\boldsymbol{x} - \boldsymbol{x}_k^{n+1})) \quad \text{where} \quad \begin{cases} \boldsymbol{x}_k^{n+1} = F^n(\boldsymbol{x}_k^n) \\ D_k^{n+1} = D_k^n J_k^n \end{cases}$$

and $J_k^n \approx (J_{F^n}(\boldsymbol{x}_k^n))^{-1} = J_{(F^n)^{-1}}(\boldsymbol{x}_k^{n+1})$. In practice, use Finite Differences

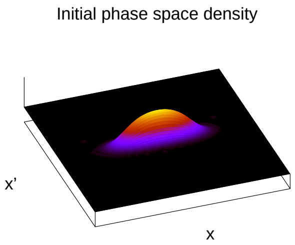
$$(\tilde{J}_k^n)_{i,j} := (2h)^{-1}\big((F^n)_i(\boldsymbol{x}_k^n + h\boldsymbol{e}_j) - (F^n)_i(\boldsymbol{x}_k^n - h\boldsymbol{e}_j)\big) \approx \partial_j(F^n)_i(\boldsymbol{x}_k^n)$$

and a "conservative" inversion $J_k^n := \det(\tilde{J}_k^n)^{\frac{1}{d}}(\tilde{J}_k^n)^{-1}$.

Outline

Illustration : mismatched thermal sheet-beam

- 1D1V model of unbunched sheet-beam propagating in constant focusing channel, phase advance $\sigma_0 = 60^\circ$ per lattice period (Lund, Friedman and Bazouin, 2011)
- Physical parameters $\sim$ consistent with NDCX-I : 100 KeV K^+ beam, tune depression $\sigma/\sigma_0 = 0.5$ and mismatch parameter $\mu = x_b/x_b^{\mathrm{eq}} = 1.25$



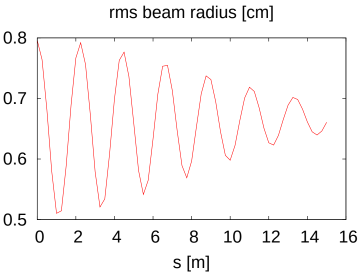


Illustration : mismatched thermal sheet-beam

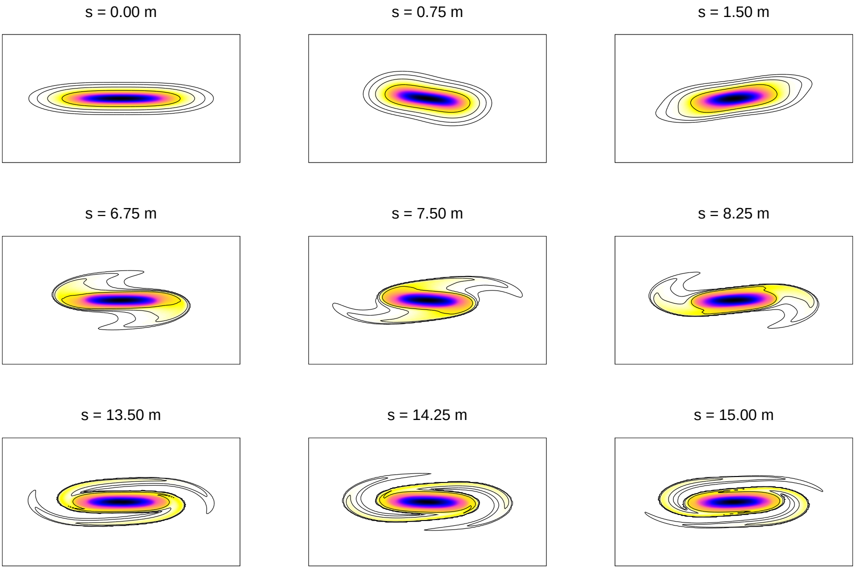
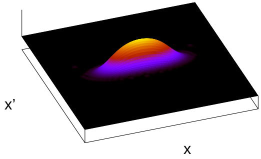


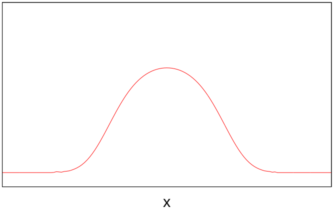
Illustration : mismatched thermal sheet-beam

- ▷ unweigthed PIC with $N_p = 64 \times 64$ particles, Poisson solved on 128 cells
- ▷ (32 particles per cell) 600 time steps for 30 lattice periods

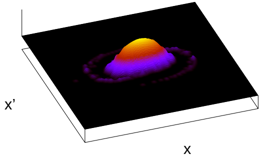
Initial phase space density



Initial charge (x) density



Final phase space density



Final charge (x) density

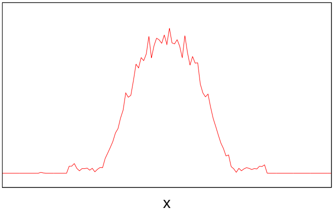
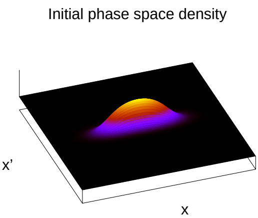
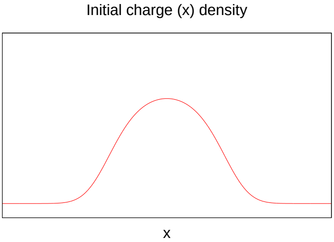


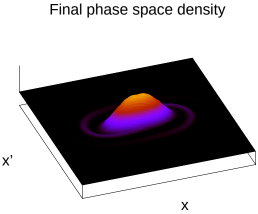
Illustration : mismatched thermal sheet-beam

▷ Cubic Bspline particles initialized on 64×64 grid, Poisson solved on 128 cells

▷ (≤ 32 particles per cell) 7 remappings in 600 time steps, for 30 lattice periods







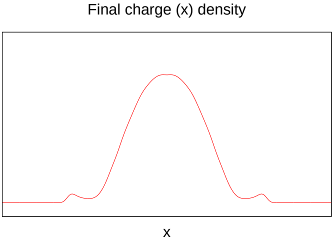


Illustration : mismatched thermal sheet-beam

▷ PIC ($p = 1$) vs LTP using Poisson solved on 128 cells and $\leq$ 32 particles per cell

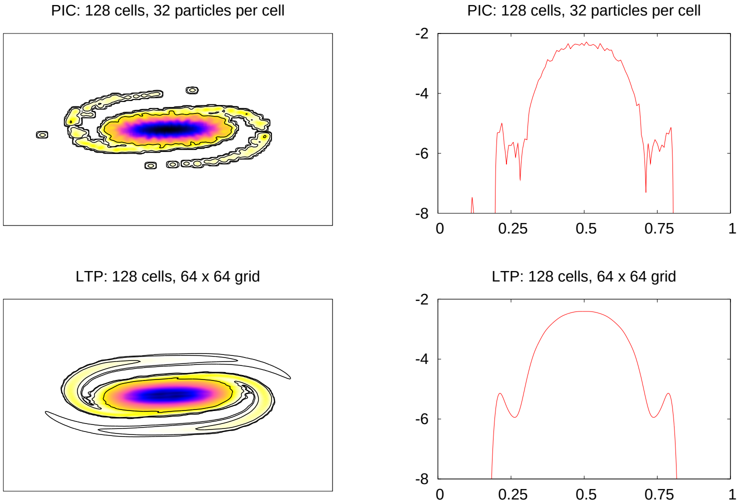
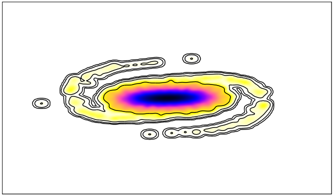


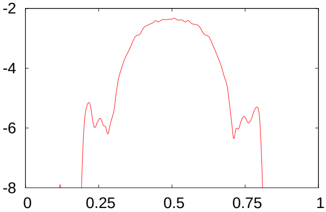
Illustration : mismatched thermal sheet-beam

▷ PIC ($p = 3$) vs LTP using Poisson solved on 128 cells and $\leq$ 32 particles per cell

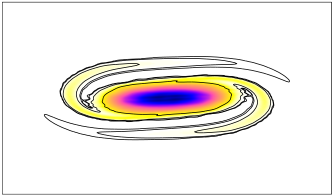
PIC_p3: 128 cells, 32 particles per cell



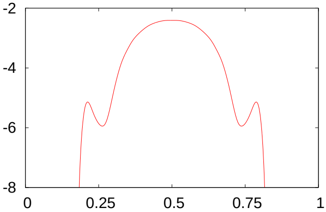
PIC_p3: 128 cells, 32 particles per cell



LTP: 128 cells, 64 x 64 grid



LTP: 128 cells, 64 x 64 grid



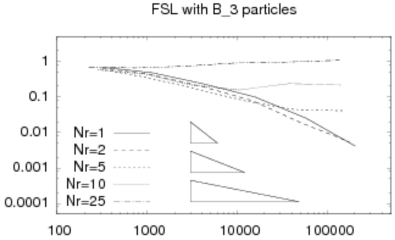
Outline

Theoretical convergence result

Question : assuming smooth data $f(t=0)$ and flows F^n, do we have

$$\max_{\boldsymbol{x}} \left| f_h^n(\boldsymbol{x}) - f(\boldsymbol{x}, t^n) \right| \to 0 \qquad \text{for} \qquad h \to 0 \quad ?$$

- For smoothed particles : yes with a "smoothing kernel" argument but requires $\varepsilon \sim h^{\alpha}$ with $\alpha < 1$ and moment condition for φ (Raviart, 1985)
- For remapped particles : it seems so (but introduces numerical dissipation)
- For deformed particles : yes, with no assumptions on φ, and no remappings



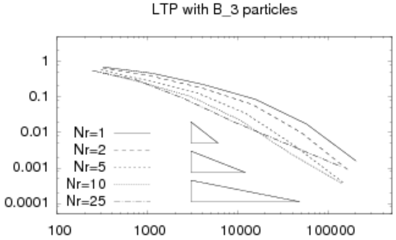
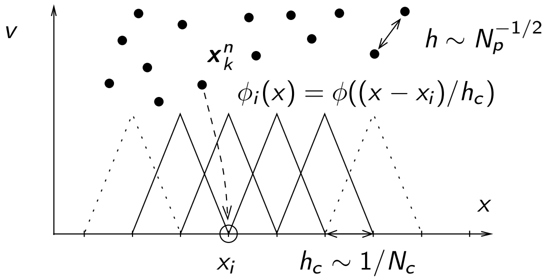


Illustration : the PIC method with linear weighting



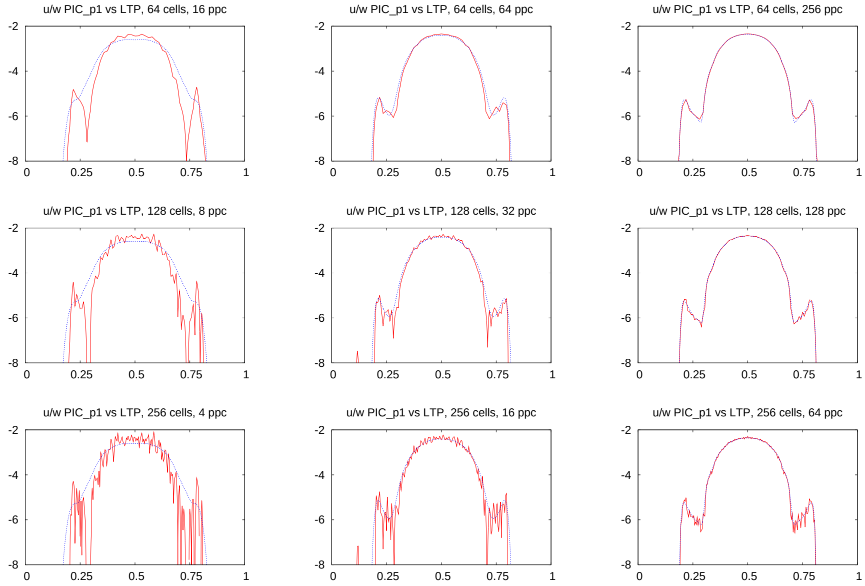
Point particles $w_k \delta_{\boldsymbol{x}_k^n}$ deposit their charge as

$$\rho_i^n = \sum_k w_k \phi_i(x_k^n) = h_c \int f_\varepsilon^n(x_i, v)\,\mathrm{d}v \quad \text{with} \quad f_\varepsilon^n(\boldsymbol{x}) := \sum_k w_k \varphi_\varepsilon(\boldsymbol{x} - \boldsymbol{x}_k^n)$$

Here the particles $\varphi_\varepsilon(x, v) = \varepsilon^{-2}\phi(\frac{x}{\varepsilon})\phi(\frac{v}{\varepsilon})$ have smoothing scale $\varepsilon = h_c$

$\implies$ convergence requires $h_c \sim h^\alpha$, hence $N_p/N_c \sim N_c^\beta$ with $\beta = \frac{2-\alpha}{\alpha} > 1$

Log plots of charge density : unweighted PIC vs LTP



Outline

Clonclusion and open questions

- New approach decouples the resolution of the transport equation (N_p) and that of the Force field (N_c)
  mapsto noiseless method, simpler to use ?
  - M. CP, A. Friedman, S. Lund and D. Grote (in preparation)
  - M. CP and S. Lund (in preparation)
- Same scaling for the particles and their initialization/remapping grid
  $\mapsto$ efficient (high order) approximation schemes, adaptive grids (as with FSL)
- New convergence analysis, more flexible than the traditional "smoothing kernel" argument
  - M. CP, *Smooth particles methods without smoothing* (in preparation)

▷ Develop a dynamic (and local) criterion for remappings

▷ Design efficient adaptive version

▷ Implement higher order methods with polynomial deformations

▷ ...